Supplementary Information File

Dissecting the role of Bi and Ba in the catalytic efficiency of VSbBiBa/Al_2O_3 catalysts n propane oxidative dehydrogenation

A. Bouzeggane[1], P.P. Bargiela[1], M. Aouine[1], R. Checa[1], I. Popescu[2], I.C. Marcu[2], O. Peruch[3], V. Bellière-Baca[3] and J.M.M. Millet[1]

[1] Univ Lyon, Université Claude Bernard Lyon 1, CNRS, IRCELYON - UMR 5256, 2 Av. Albert Einstein, 69626 Villeurbanne, France

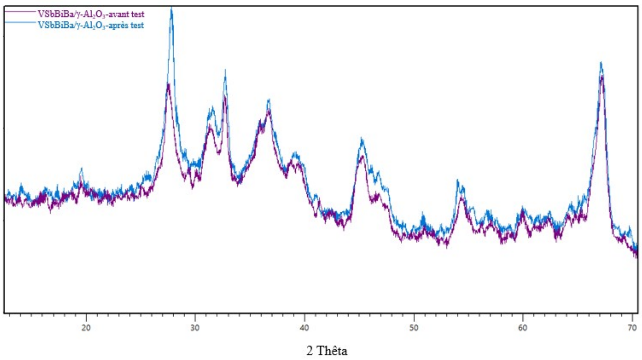

Figure S1 : X-ray diffractogram of the VSbBiBaO/γ-Al_2O_3 catalyst before (blue) and after 24 h of catalytic test (purple).

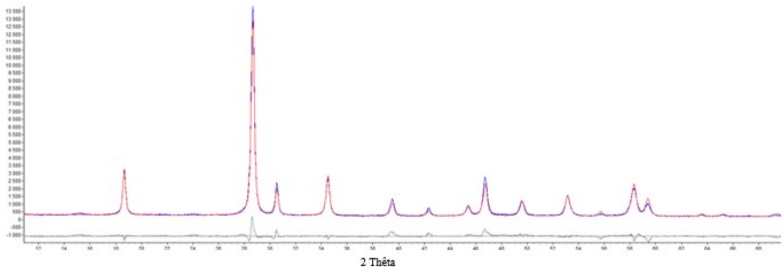

Figure S2 : Final Rietveld plot for the $VSb_{0.9}Bi_{0.1}O_4$ sample with in red the observed data and in blue the computed ones; the bottom grey line corresponds to the difference curve.

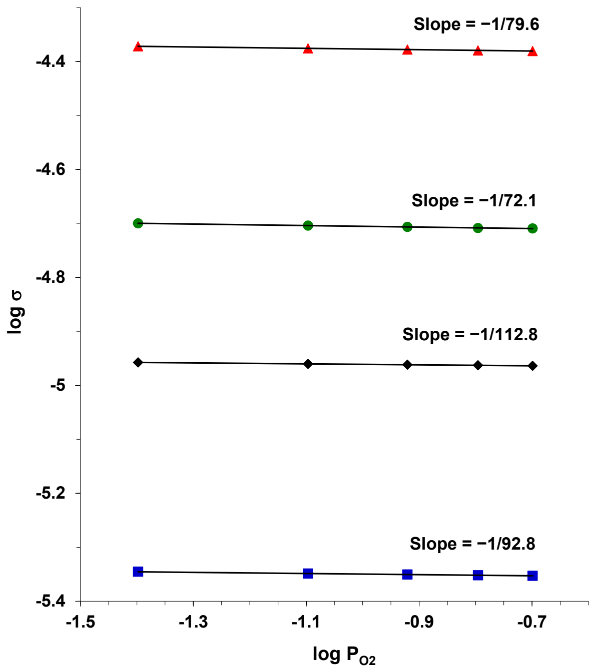

Figure S3 : Variation of σ as a function of the oxygen pressure for $VSbO_4$ (◆) and $VBi_xSb_{1-x}O_4$ samples with *x* = 0.05 (○), 0.08 (□) and 0.1 (℘), at 350 °C in a log–log plot (P_{O_2} in atm; σ in ohm^{-1} cm^{-1}).

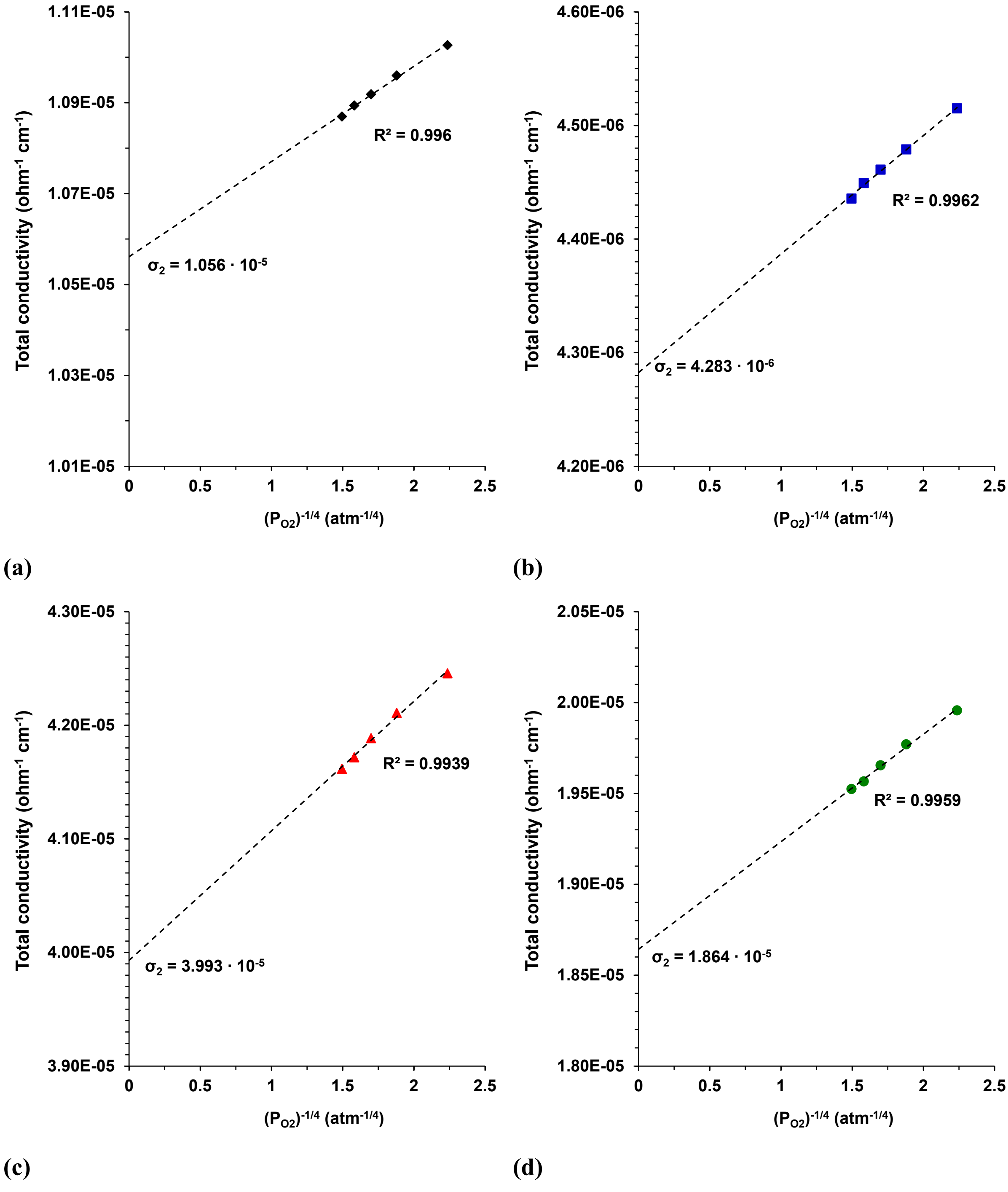

Figure S4 : Total conductivity, σ, as a function of $P_{O_2}^{-1/4}$ at 350 °C for $VSbO_4$ (a) and $VBi_xSb_{1-x}O_4$ mixed oxides with x = 0.05 (b), 0.08 (c) and 0.1 (d).

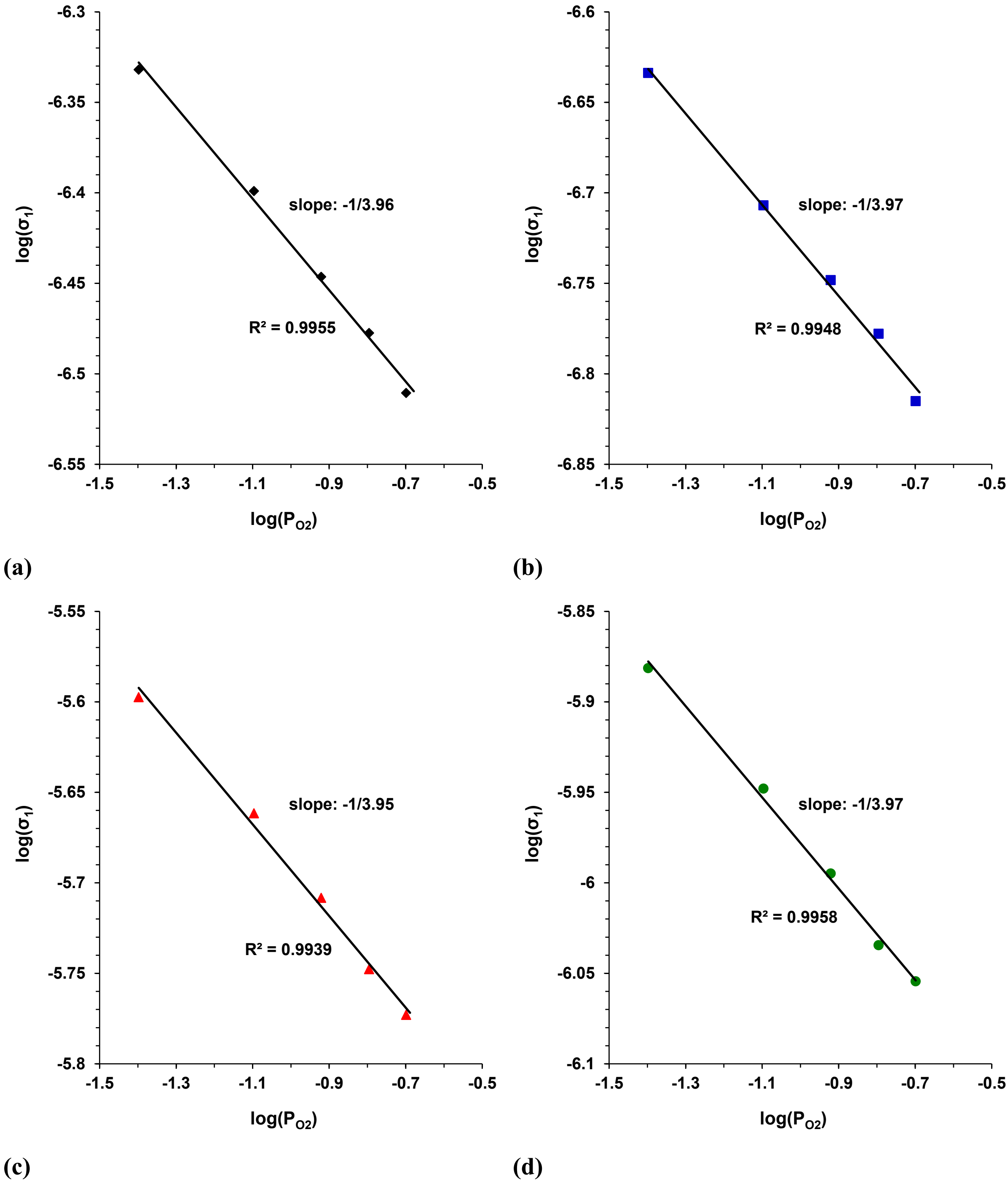

Figure S5 : σ_1 conductivity as a function of the oxygen pressure in a log–log plot at 350 °C for $VSbO_4$ (a) and $VBi_xSb_{1-x}O_4$ mixed oxides with x = 0.05 (b), 0.08 (c) and 0.1 (d).

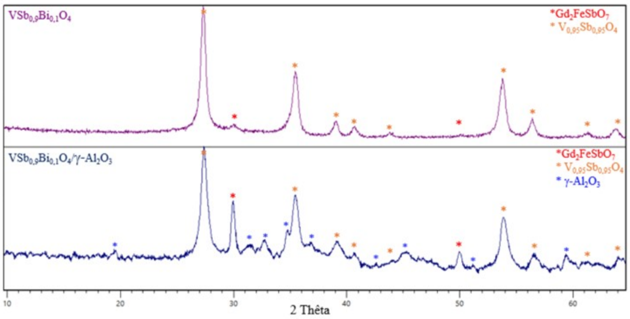

Figure S6 : X-ray diffraction patterns of the catalysts synthesized under microwaves without ($VSb_{0.9}Bi_{0.1}O_4$) and with alumina ($VSb_{0.9}Bi_{0.1}O_4 + Al_2O_3$).

Table S1: Catalytic properties of the $VSbBiBaO/Al_2O_3$ catalyst in the oxidation of propane. Catalyst was first tested at 380°C for comparison with other catalysts (Table 1) and then at 400°C in different conditions in order to avoid total conversion of O_2. The test was then conducted at 350°C in the same conditions as at 400°C.

Temperature (°C)	Conv. (%)		Selectivity (%)						Yield (%)	
	C_3H_8	O_2	$C_3H_{6.}$	ACRO	ACRY	Others	CO	CO_2	C_3H_6	C_3H_6+ACRO
350	17	86	21	6	2	1	32	38	3.5	4.6
380	22.7	97	16	3	1	-	42	48	3.6	4.3
400	27	99	15	4	2	-	44	35	4.1	5.1

Notes: Reaction conditions at 350 and 400°C : C_3H_8/O_2/10%Ne-He 1/1/8, Total flow = 20 ml.min^{-1}, GHSV=2000ml.g^{-1}.h^{-1}; reaction conditions at 380°C C_3H_8/O_2/10%Ne-He 10/8.7/8, Total flow]= 25ml.min^{-1} GHSV=2500 ml.g^{-1}.h^{-1}. ; ACRO : acrolein, ACRY: acrylic acid, others* : acetic acid and acetaldehyde.